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Application of a Synthesis and Design Methodology to achieve Process Intensification

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In recent years, Process Intensification (PI) has attracted considerable academic interest as a potential means of process improvement, to meet the increasing demands for sustainable production. PI aims to benefit processes without sacrificing product quality by increasing efficiency, reducing energy consumption, costs, volume, and waste as well as improving safety. A variety of intensified operations and equipment has been developed in academia and industry. Potentially, this creates a large number of options to improve the process but to date only a limited number have achieved implementation in industry, such as reactive distillation, dividing wall columns and reverse flow reactors [1].

Some of the reasons for this are that the currently available methods/ techniques to decide where, when and how to intensify the process under investigation for the maximal improvement of a target is neither simple nor systematic and take considerable resources. Hence, a process synthesis tool to achieve PI would potentially assist in the generation and evaluation of PI options. This leads to the development of a general PI synthesis and design methodology based on the decomposition approach for the mathematical optimization problem in which the lower level steps employ simple and easy calculations, while the higher level steps employ more rigorous and detailed calculations [2]. First, the synthesis/ design problem has to be carefully defined in terms of objective, scenario and constraints to be solved. Additionally, a performance metric for screening process options are selected. Afterwards, information of the process, components and reactions are collected and analyzed for identification of limitations/ bottlenecks of the process. These can be linked to phenomena which need intensification to improve the process. Based on this knowledge, PI strategies are identified which potentially improve the process under investigation. Necessary models to represent the process are either developed or retrieved from a model library. Through synthesis rules new processes options are generated which are screened by logical and structural constraints in order to ensure the quantity and quality of the product, redundant options are removed. Through short-cut models, the performance of each option is determined, and redundant options with respect to operational constraints are removed. The most promising remaining options determined by performance metric are finally optimized, and validated through rigorous simulations and/ or experiments. Such a methodology is reliant on a set of tools as well as structured knowledge, which is provided in this work through retrieval from a computer-aided knowledge base in which relevant knowledge of PI technologies is stored.

In this paper the application of the systematic methodology through the whole computer-aided framework will be described and highlighted with selected examples of industrial importance.

- [1] Harmsen, J. Process Intensification in the petrochemicals industry: Drivers and hurdles for commercial implementation. *Chem Eng Process* 2010; 49: 70-73.
- [2] Lutze, P., Gani, R., Woodley. Process intensification: A perspective on process synthesis. *Chem Eng Process* 2010; 49: 547-558.